Ferromagnetic phases in spin-Fermion systems

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Spin-Fermion systems which obtain their magnetic properties from a system of localized magnetic moments being coupled to conducting electrons are considered. The dynamical degrees of freedom are spin-s operators of localized spins and spin-1/2 Fermi operators of itinerant electrons. Renormalized spin-wave theory, which accounts for the magnon-magnon interaction, and its extension are developed to describe the two ferrimagnetic phases in the system: low temperature phase $0 < T < T^*$, where all electrons contribute the ordered ferromagnetic moment, and high temperature phase $T^* < T < T_C$, where only localized spins form magnetic moment. The magnetization as a function of temperature is calculated. The theoretical predictions are utilize to interpret the experimentally measured magnetization-temperature curves of UGe_2..

I. INTRODUCTION

Spin-Fermion systems, which obtain their magnetic properties from a system of localized magnetic moments and itinerant electrons are considered. The true magnons in these systems, which are the transversal fluctuations corresponding to the total magnetization, are complicated mixtures of the transversal fluctuations of the spins of localized and itinerant electrons[1]. The magnons interact with localized magnetic moments and itinerant electrons in a different way. Magnons' fluctuations suppress the ordered moments of the localized and itinerant electrons at different temperatures. As a result, the ferromagnetic phase is divided into two phases: low temperature phase $0 < T < T^*$, where all electrons contribute the ordered ferromagnetic moment, and high temperature phase $T^* < T < T_C$, where only localized spins form magnetic moment.

At first sight the result seems to be counterintuitive because the moment formed by localized electrons builds an effective magnetic field, which due to exchange interaction leads to a finite magnetization of the itinerant electrons. This is true in the classical limit. In the quantum case the spin wave fluctuations suppress the magnetic orders at different temperatures T^* and T_C as a result of a different interaction of magnons with the localized and itinerant electrons. The T^* transition is a transition between two magnetically-ordered phases in contrast to the transition from the magnetically ordered state to the paramagnetic one (T_C-transition).

First approach to itinerant electron magnetism, which accounts for the spin fluctuations, has been developed by Moriya and Kawabata [2, 3]. It is a self-consistent one loop approximation which interpolates between the Heisenberg theory of localized spins and theory of nearly ferromagnetic metals. The nonlinear effects of spin fluctuations are treated in [4], using a self-consistent rotationally invariant Hartree approximation for itinerant electrons' interaction.

In the spin-Fermion systems the localized spins polarize the itinerant electrons and that feeds back as an indirect coupling between the localized spins. Averaging in the subspace of the itinerant electrons, one obtains an effective Heisenberg like model in terms of the localized spins. This indirect exchange coupling is referred to as Rudermann-Kittel-Kasuya-Yosida (RKKY) interaction [5–7]. An approximate but self-consistent theory of spin-Fermion systems is presented in [8]. In second-order perturbation theory one gets the well-known RKKY effective interection. The magnetization curve, the spin polarization of the itinerant electrons and the correlation functions are worked out in terms of the band occupation and exchange coupling. The subtle point is that the transversal spin fluctuations are not the true magnon of the system. Therefore the RKKY validity condition requires not only small Kondo coupling, but it also requires the charge carrier density to be small, which in turn means that the magnetization of the mobile electrons is inessential.

In the present paper the Schwinger bosons and slave Fermions are introduced to separate the spin fluctuations of the electrons from the charge ones. The slave Fermions, which are spinless, are integrated out and an effective model in terms of the transversal fluctuations of the spins of localized and itinerant electrons is obtained. The anomaly results from the existence of the two separated sources of magnetization.

Renormalized spin-wave (RSW) theory, which accounts for the magnon-magnon interaction, and its extension are developed to describe the two ferromagnetic phases in the system and to calculate the magnetization as a function of temperature. It is impossible to require the theoretically calculated Curie temperature and magnetization-temperature curves to be in exact accordance with experimental results. The models are idealized, and they do not consider many important effects. Because of this it is important to formulate theoretical criteria for adequacy of the method of calculation. In my opinion the calculations should be in accordance with the Mermin-Wagner theorem [9]. It claims that at nonzero temperature, a one-dimensional or two-dimensional isotropic spin-S Heisenberg model with finite-range exchange interaction can be neither ferro-

magnetic nor antiferromagnetic. The present method of calculation, being approximate, captures the essentials of the magnon fluctuations in the theory and satisfy the Mermin-Wagner theorem. The physics of the ferromagnetic spin-Fermion systems is dominated by the magnon fluctuations and it is important to account for them in the best way. Comparing figure 4 in the present paper and figure 2 in [1] one becomes aware of the relevance of the present calculations for the accurate reproduction of the basic features of the system near the characteristic temperatures T_C and T^*.

To compare the theoretical results and the experimental magnetization-temperature curves one has, first of all, to interpret adequately the measurements. As an example, the experimental measurements of the ferromagnetic phase of UGe_2 are considered . They reveal the presence of an additional phase line that lies entirely within the ferromagnetic phase. The characteristic temperature of this transition T_x, which is below the Curie temperature T_C, decreases with pressure and disappears at a pressure close to the pressure at which new phase of coexistence of superconductivity and ferromagnetism emerges[10–12]. The additional phase transition demonstrates itself through the change in the T dependence of the ordered ferromagnetic moment[13–15]. The magnetization shows an anomalous enhancement below T_x.

The paper is organized as follows. In Sec. II an effective model in terms of the transversal fluctuations of the spins of localized and itinerant electrons is obtained. In Sec. III a renormalized spin-wave theory is worked out to calculate the magnetization-temperature curve. The analysis of the experimental magnetization-temperature curves is given in Sec. IV. To study the magnetic properties of the UGe_2 an effective two magnetic ordered moments model is considered. Varying the model's parameters, the anomalous temperature dependence of the magnetization, known from the experiments with UGe_2 [11, 13–15], are reproduced theoretically. It is shown that the experimentally measured transition at temperature $T_x(=T^*)$ is a transition from high temperature phase $T^* < T < T_C$, where only part of the $5f$ uraniun electrons contribute the ordered ferromagnetic moment, to low temperature phase $0 < T < T^*$, where all electrons contribute the magnetization. A summary in Sec. V concludes the paper.

II.   EFFECTIVE MODEL

The dynamical degrees of freedom in spin-Fermion model are spin-s operators of localized spins and spin-$1/2$ Fermi operators of itinerant electrons. One considers a theory with Hamiltonian

$$h = H - \mu N = -t \sum_{\langle ij \rangle} \left(c_{i\sigma}^+ c_{j\sigma} + h.c. \right) - \mu \sum_i n_i$$

$$- J^l \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J' \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j - J \sum_i \mathbf{S}_i \cdot \mathbf{s}_i \quad (1)$$

where $s_i^\nu = \frac{1}{2} \sum_{\sigma\sigma'} c_{i\sigma}^+ \tau_{\sigma\sigma'}^\nu c_{i\sigma'}$, with the Pauli matrices (τ^x, τ^y, τ^z), is the spin of the conduction electrons, $\mathbf{S}_i$ is the spin of the localized electrons, μ is the chemical potential, and $n_i = c_{i\sigma}^+ c_{i\sigma}$. The sums are over all sites of a three-dimensional cubic lattice, and $\langle i, j \rangle$ denotes the sum over the nearest neighbors. The Heisenberg terms describe ferromagnetic Heisenberg exchange between nearest-neighbors localized ($J^l > 0$) and itinerant ($J' > 0$) electrons. The last term in Eq.(1) describes the ferromagnetic spin-Fermion interaction ($J > 0$).

One represents the Fermi operators in terms of the Schwinger bosons $(\varphi_{i,\sigma}, \varphi_{i,\sigma}^+)$ and slave Fermions (h_i, h_i^+, d_i, d_i^+)[1]. The Bose fields are doublets ($\sigma = 1, 2$) without charge, while Fermions are spinless with charges 1 (d_i) and -1 (h_i).

$$c_{i\uparrow} = h_i^+ \varphi_{i1} + \varphi_{i2}^+ d_i, \qquad c_{i\downarrow} = h_i^+ \varphi_{i2} - \varphi_{i1}^+ d_i,$$

$$n_i = 1 - h_i^+ h_i + d_i^+ d_i, \quad s_i^\nu = \frac{1}{2} \sum_{\sigma\sigma'} \varphi_{i\sigma}^+ \tau_{\sigma\sigma'}^\nu \varphi_{i\sigma'},$$

$$\varphi_{i1}^+ \varphi_{i1} + \varphi_{i2}^+ \varphi_{i2} + d_i^+ d_i + h_i^+ h_i = 1 \quad (2)$$

Next, we make a change of variables, introducing Bose doublets $\zeta_{i\sigma}$ and $\zeta_{i\sigma}^+$ [16]

$$\zeta_{i\sigma} = \varphi_{i\sigma} \left(1 - h_i^+ h_i - d_i^+ d_i \right)^{-\frac{1}{2}},$$

$$\zeta_{i\sigma}^+ = \varphi_{i\sigma}^+ \left(1 - h_i^+ h_i - d_i^+ d_i \right)^{-\frac{1}{2}}, \quad (3)$$

where the new fields satisfy the constraint $\zeta_{i\sigma}^+ \zeta_{i\sigma} = 1$. In terms of the new fields the spin vectors of the itinerant electrons have the form

$$s_i^\nu = \frac{1}{2} \sum_{\sigma\sigma'} \zeta_{i\sigma}^+ \tau_{\sigma\sigma'}^\nu \zeta_{i\sigma'} \left[1 - h_i^+ h_i - d_i^+ d_i \right], \quad (4)$$

where the unit vector $n_i^\nu = \sum_{\sigma\sigma'} \zeta_{i\sigma}^+ \tau_{\sigma\sigma'}^\nu \zeta_{i\sigma'}$ ($\mathbf{n}_i^2 = 1$) identifies the local orientation of the spin of the itinerant electron[1]. Let us average the spin of electrons in the subspace of the Fermions (d_i^+, d_i) and (h_i^+, h_i) (to integrate the Fermions out in the path integral approach). One obtains

$$\mathbf{s}_i = m\mathbf{n}_i \qquad \mathbf{s}_i^2 = m^2 \quad (5)$$

$$m = \frac{1}{2} \left(1 - <h_i^+ h_i>_f - <d_i^+ d_i>_f \right),$$

where $< ..... >_f$ means an average in the subspace of the Fermions $d(d^+)$ and $h(h^+)$ when the spin fluctuations of the itinerant electrons are set equal to zero. Hence, the amplitude of the spin vector "m" is an effective spin of the itinerant electrons accounting for the fact that some sites, in the ground state, are doubly occupied or empty.

It is more convenient to use the rescaled Bose fields

$$\xi_{i\sigma} = \sqrt{2m}\, \zeta_{i\sigma}, \qquad \xi_{i\sigma}^+ = \sqrt{2m}\, \zeta_{i\sigma}^+ \quad (6)$$

which satisfy the constraint $\xi_{i\sigma}^+ \xi_{i\sigma} = 2m$, and to introduce the vector,

$$M_i^\nu = \frac{1}{2} \sum_{\sigma\sigma'} \xi_{i\sigma}^+ \tau_{\sigma\sigma'}^\nu \xi_{i\sigma'} \quad \mathbf{M}_i^2 = m^2. \quad (7)$$

Then, the spin-vector of itinerant electrons can be written in the form

$$\mathbf{s}_i = \frac{1}{2m}\mathbf{M}_i \left(1 - h_i^+ h_i - d_i^+ d_i\right) \tag{8}$$

and $\mathbf{M_i} = <\mathbf{s}_i>_f$

The Hamiltonian is quadratic with respect to the Fermions d_i, d_i^+ and h_i, h_i^+, and one can average in the subspace of these Fermions (to integrate them out in the path integral approach). As a result, we obtain an effective theory of two vectors $\mathbf{S}_i$ and $\mathbf{M}_i$ with Hamiltonian

$$h_{eff} = -J^l \sum_{\langle ij \rangle} \mathbf{S}_i \cdot \mathbf{S}_j - J^{it} \sum_{\langle ij \rangle} \mathbf{M}_i \cdot \mathbf{M}_j - J \sum_i \mathbf{S}_i \cdot \mathbf{M}_i \tag{9}$$

The first term is the term which describes the exchange of localized spins in the Hamiltonian Eq.(1). The second term has two components: one is the term in the Hamiltonian Eq.(1) which describes the exchange of the spins of the itinerant electrons, while the second one is obtained integrating out the Fermions. It is calculated in the one loop approximation and in the limit when the frequency and the wave vector are small. For the effective exchange constant J^{it}, at zero temperature, one obtains

$$J^{it} = J' \tag{10}$$

$$+ \frac{t}{6m^2}\frac{1}{N}\sum_k \left(\sum_{\nu=1}^{3}\cos k_\nu\right)\left[\theta(-\varepsilon_k^d) - \theta(-\varepsilon_k^h)\right]$$

$$- \frac{2t^2}{3m^2 sJ}\frac{1}{N}\sum_k \left(\sum_{\nu=1}^{3}\sin^2 k_\nu\right)\left[1 - \theta(-\varepsilon_k^h) - \theta(-\varepsilon_k^d)\right]$$

where N is the number of lattice's sites, ε_k^h and ε_k^d are Fermions' dispersions,

$$\varepsilon_k^h = 2t(\cos k_x + \cos k_y + \cos k_z) + sJ/2 + \mu \tag{11}$$
$$\varepsilon_k^d = -2t(\cos k_x + \cos k_y + \cos k_z) + sJ/2 - \mu,$$

and wave vector k runs over the first Brillouin zone of a cubic lattice. Calculating the ratio J^{it}/J from the equation (10) one obtains that the second term, which comes from the tadpole diagram with one d or h line, is proportional to t/J and the last term, which results from the calculation of loop diagrams with two d or h lines is proportional to $(t/J)^2$. This means that our one loop approximation is most relevant for small t/J. For the case of experimental interest the density of itinerant electrons per lattice site is equal to one and then the contribution of the spin-Fermion interaction to the exchange constant J^{it} Eq.(10) is negative. As a result J^{it} is positive but very small compare with J^l and J. The third term in Eq.(9) is obtained from the last one in the Hamiltonian Eq.(1) using the representation Eq.(8) for the spin of itinerant electrons and Eq.(5).

III. RENORMALIZED SPIN-WAVE THEORY

We are going to study the ferromagnetic phase of the two-spin system Eq.(9) with $J^l > 0$, $J^{it} > 0$, and $J > 0$.

To proceed we use the Holstein-Primakoff representation of the spin vectors $\mathbf{S}_j(a_j^+, a_j)$ and $\mathbf{M}_j(b_j^+, b_j)$

$$S_j^+ = S_j^1 + iS_j^2 = \sqrt{2s - a_j^+ a_j}\ a_j$$
$$S_j^- = S_j^1 - iS_j^2 = a_j^+ \sqrt{2s - a_j^+ a_j}$$
$$S_j^3 = s - a_j^+ a_j \tag{12}$$
$$M_j^+ = M_j^1 + iM_j^2 = \sqrt{2m - b_j^+ b_j}\ b_j$$
$$M_j^- = M_j^1 - iM_j^2 = b_j^+ \sqrt{2m - b_j^+ b_j}$$
$$M_j^3 = m - b_j^+ b_j$$

where a_j^+, a_j and b_j^+, b_j are Bose fields, while s and m are the effective spins of the localized and itinerant electrons. In terms of the Bose fields and keeping only the quadratic and quartic terms, the effective Hamiltonian Eq.(9) adopts the form

$$h_{eff} = h_2 + h_4 \tag{13}$$

where

$$h_2 = sJ^l \sum_{\langle ij \rangle}(a_i^+ a_i + a_j^+ a_j - a_j^+ a_i - a_i^+ a_j)$$

$$+ mJ^{it}\sum_{\langle ij \rangle}(b_i^+ b_i + b_j^+ b_j - b_j^+ b_i - b_i^+ b_j) \tag{14}$$

$$- J\sum_i(\sqrt{sm}\,[a_i^+ b_i + b_i^+ a_i] - sb_i^+ b_i - ma_i^+ a_i)$$

$$h_4 = \frac{J^l}{4}\sum_{\langle ij \rangle}[a_i^+ a_j^+(a_i - a_j)^2 + (a_i^+ - a_j^+)^2 a_i a_j]$$

$$+ \frac{J^{it}}{4}\sum_{\langle ij \rangle}[b_i^+ b_j^+(b_i - b_j)^2 + (b_i^+ - b_j^+)^2 b_i b_j]$$

$$+ \frac{J}{4}\sum_i[\sqrt{\frac{s}{m}}(a_i^+ b_i^+ b_i b_i + b_i^+ b_i^+ b_i a_i) \tag{15}$$

$$+ \sqrt{\frac{m}{s}}(b_i^+ a_i^+ a_i a_i + a_i^+ a_i^+ a_i b_i) - 4a_i^+ a_i b_i^+ b_i]$$

and terms without fields are dropped.

The next step is to represent the Hamiltonian in the Hartree-Fock approximation:

$$h_{eff} \approx h_{HF} = h_{cl} + h_q \tag{16}$$

where

$$h_{cl} = 3NJ^l s^2(u^l - 1)^2 + 3NJ^{it}m^2(u^{it} - 1)^2$$
$$+ NJsm(u - 1)^2, \tag{17}$$

$$h_q = sJ^l u^l \sum_{\langle ij \rangle}(a_i^+ a_i + a_j^+ a_j - a_j^+ a_i - a_i^+ a_j)$$

$$+ mJ^{it}u^{it}\sum_{\langle ij \rangle}(b_i^+ b_i + b_j^+ b_j - b_j^+ b_i - b_i^+ b_j) \tag{18}$$

$$- Ju\sum_i(\sqrt{sm}\,[a_i^+ b_i + b_i^+ a_i] - sb_i^+ b_i - ma_i^+ a_i)$$

Equation (18) shows that the Hartree-Fock parameters u^l, u^{it} and u renormalize the exchange constants J^l, J^{it} and J, respectively.

It is convenient to rewrite the Hamiltonian in the momentum space representation:

$$h_q = \sum_k \left(\varepsilon_k^a a_k^+ a_k + \varepsilon_k^b b_k^+ b_k - \gamma \left(a_k^+ b_k + b_k^+ a_k \right) \right),$$
(19)

where the wave vector k runs over the first Brillouin zone B of a cubic lattice. The dispersions are given by the equalities

$$\begin{aligned} \varepsilon_k^a &= 2s\, J^l\, u^l \varepsilon_k + m\, J u \\ \varepsilon_k^b &= 2m\, J^{it}\, u^{it} \varepsilon_k + s\, J u \\ \gamma &= J u \sqrt{s\, m} \end{aligned}$$
(20)

with

$$\varepsilon_k = 3 - \cos k_x - \cos k_y - \cos k_z.$$
(21)

To diagonalize the Hamiltonian, one introduces new Bose fields α_k, α_k^+, β_k, β_k^+,

$$\begin{aligned} a_k &= \cos\theta_k\, \alpha_k + \sin\theta_k\, \beta_k, \\ b_k &= -\sin\theta_k\, \alpha_k + \cos\theta_k\, \beta_k \end{aligned}$$
(22)

with coefficients of transformation,

$$\cos\theta_k = \sqrt{\frac{1}{2}\left(1 + \frac{\varepsilon_k^a - \varepsilon_k^b}{\sqrt{(\varepsilon_k^a - \varepsilon_k^b)^2 + 4\gamma^2}}\right)},$$
(23)
$$\sin\theta_k = \sqrt{\frac{1}{2}\left(1 - \frac{\varepsilon_k^a - \varepsilon_k^b}{\sqrt{(\varepsilon_k^a - \varepsilon_k^b)^2 + 4\gamma^2}}\right)}$$

The transformed Hamiltonian adopts the form

$$h_q = \sum_k \left(E_k^\alpha \alpha_k^+ \alpha_k + E_k^\beta \beta_k^+ \beta_k \right),$$
(24)

with new dispersions

$$\begin{aligned} E_k^\alpha &= \frac{1}{2}\left[\varepsilon_k^a + \varepsilon_k^b + \sqrt{(\varepsilon_k^a - \varepsilon_k^b)^2 + 4\gamma^2} \right] \\ E_k^\beta &= \frac{1}{2}\left[\varepsilon_k^a + \varepsilon_k^b - \sqrt{(\varepsilon_k^a - \varepsilon_k^b)^2 + 4\gamma^2} \right] \end{aligned}$$
(25)

With positive exchange constants J^l, J^{it}, J and positive Hartree-Fock parameters u^l, u^{it}, u the Bose fields' dispersions are positive $\varepsilon_k^a > 0$, $\varepsilon_k^b > 0$ for all values of $k \in B$. As a result, $E_k^\alpha > 0$ and $E_k^\beta \geq 0$ with $E_0^\beta = 0$.

Near the zero wave vector, $E_k^\beta \approx \rho k^2$ where the spin-stiffness constant is

$$\rho = \frac{(s^2 J^l u^l + m^2 J^{it} u^{it})}{(s + m)}.$$
(26)

Hence, β_k is the long-range (**magnon**) excitation in the two-spin effective theory, while α_k is a gapped excitation with gap $E_0^\alpha = (s + m)Ju$.

To obtain the system of equations for the Hartree-Fock parameters we consider the free energy of a system with Hamiltonian h_{HF} equations (16), (17) and (24):

$$\mathcal{F} = 3J^l s^2 (u^l - 1)^2 + 3J^{it} m^2 (u^{it} - 1)^2 + Jsm(u - 1)^2$$
(27)
$$+ \frac{1}{\beta N} \sum_k \left[\ln\left(1 - e^{-\beta E_k^\alpha}\right) + \ln\left(1 - e^{-\beta E_k^\beta}\right) \right],$$

where $\beta = 1/T$ is the inverse temperature. Then the three equations for the Hartree-Fock parameters

$$\partial\mathcal{F}/\partial u^l = 0, \quad \partial\mathcal{F}/\partial u^{it} = 0, \quad \partial\mathcal{F}/\partial u = 0$$
(28)

have the form (see the appendix)

$$u^l = 1 - \frac{1}{3s}\frac{1}{N}\sum_k \varepsilon_k \left[\cos^2\theta_k\, n_k^\alpha + \sin^2\theta_k\, n_k^\beta\right]$$

$$u^{it} = 1 - \frac{1}{3m}\frac{1}{N}\sum_k \varepsilon_k \left[\sin^2\theta_k\, n_k^\alpha + \cos^2\theta_k\, n_k^\beta\right]$$

$$u = 1 - \frac{1}{N}\sum_k \left[\left(\frac{1}{2s}\cos^2\theta_k + \frac{1}{2m}\sin^2\theta_k\right) n_k^\alpha \right.$$
$$+ \left(\frac{1}{2m}\cos^2\theta_k + \frac{1}{2s}\sin^2\theta_k\right) n_k^\beta$$
(29)
$$\left. + \frac{Ju}{\sqrt{(\varepsilon_k^a - \varepsilon_k^b)^2 + 4\gamma^2}}\, (n_k^\alpha - n_k^\beta)\right]$$

where n_k^α and n_k^β are the Bose functions of α_k and β_k excitations. The Hartree-Fock parameters, the solution of the system of equations (29), are positive functions of T/J, $u^l(T/J) > 0$, $u^{it}(T/J) > 0$ and $u(T/J) > 0$. Utilizing these functions, one can calculate the spontaneous magnetization of the system, which is a sum of the spontaneous magnetization of the localized and itinerant electrons $M = M^l + M^{it}$. In terms of the Bose functions of the α_k and β_k excitations they adopt the form

$$M^l = s - \frac{1}{N}\sum_k \left[\cos^2\theta_k\, n_k^\alpha + \sin^2\theta_k\, n_k^\beta\right],$$

$$M^{it} = m - \frac{1}{N}\sum_k \left[\sin^2\theta_k\, n_k^\alpha + \cos^2\theta_k\, n_k^\beta\right],$$

$$M = s + m - \frac{1}{N}\sum_k \left[n_k^\alpha + n_k^\beta\right].$$
(30)

The magnetization depends on the dimensionless temperature T/J and dimensionless parameters s, m, J^l/J and

J^{it}/J. For parameters $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$ the functions $M^l(T/J)$ and $M^{it}(T/J)$ are depicted in figure 1. The upper (black) line is the magnetization of the localized electrons M^l, the bottom (red) line is the magnetization of the itinerant electrons M^{it}.
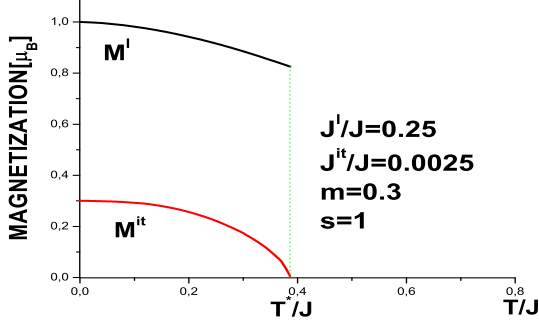

FIG. 1: (color online) Temperature dependence of the spontaneous magnetization for parameters $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$: M^l (black line)-magnetization of the localized electrons, M^{it} (red line)-magnetization of the itinerant electrons. T^* is the temperature at which the magnetization of the itinerant electrons becomes equal to zero

At characteristic temperature T^* spontaneous magnetization of itinerant electrons becomes equal to zero, while spontaneous magnetization of localized spins is still nonzero. This is because the magnon excitation β_k in the effective theory Eq.(9) is a complicated mixture of the transversal fluctuations of the spins of localized and itinerant electrons Eq.(22). As a result, the magnons' fluctuations suppress in a different way the magnetic order of these electrons. Above T^* the system of equations (29) has no solution and one has to modify the renormalized spin-wave theory.

A. Modified RSW theory

To formulate mathematically the modified RSW theory one introduces [1] two parameters λ^l and λ^{it} to enforce the magnetic moments both of the localized and the itinerant electrons to be equal to zero in paramagnetic phase. To this end, we add two new terms to the effective Hamiltonian Eq.(9),

$$\hat{h}_{eff} = h_{eff} - \sum_i \left[\lambda^l S_i^z + \lambda^{it} M_i^z\right]. \qquad (31)$$

In Hartree-Fock approximation, in momentum space, the Hamiltonian adopts the form

$$\hat{h}_q = \sum_k \left(\hat{\varepsilon}_k^a a_k^+ a_k + \hat{\varepsilon}_k^b b_k^+ b_k - \gamma\left(a_k^+ b_k + b_k^+ a_k\right)\right), \qquad (32)$$

where the the new dispersions are

$$\hat{\varepsilon}_k^a = \varepsilon_k^a + \lambda^l, \qquad \hat{\varepsilon}_k^b = \varepsilon_k^b + \lambda^{it}. \qquad (33)$$

Utilizing the same transformation Eq.(22) with coefficients

$$\cos\hat{\theta}_k = \sqrt{\frac{1}{2}\left(1 + \frac{\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b}{\sqrt{(\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b)^2 + 4\gamma^2}}\right)}, \qquad (34)$$

$$\sin\hat{\theta}_k = \sqrt{\frac{1}{2}\left(1 - \frac{\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b}{\sqrt{(\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b)^2 + 4\gamma^2}}\right)}$$

one obtains the Hamiltonian in diagonal form

$$\hat{h}_q = \sum_k \left(\hat{E}_k^\alpha \alpha_k^+ \alpha_k + \hat{E}_k^\beta \beta_k^+ \beta_k\right), \qquad (35)$$

where

$$\hat{E}_k^\alpha = \frac{1}{2}\left[\hat{\varepsilon}_k^a + \hat{\varepsilon}_k^b + \sqrt{(\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b)^2 + 4\gamma^2}\right]$$

$$\hat{E}_k^\beta = \frac{1}{2}\left[\hat{\varepsilon}_k^a + \hat{\varepsilon}_k^b - \sqrt{(\hat{\varepsilon}_k^a - \hat{\varepsilon}_k^b)^2 + 4\gamma^2}\right]. \qquad (36)$$

It is convenient to represent the parameters λ^l and λ^{it} in the form

$$\lambda^l = mJ(\mu^l - 1), \qquad \lambda^{it} = sJ(\mu^{it} - 1). \qquad (37)$$

In terms of the parameters μ^l and μ^{it}, the dispersions adopt the form

$$\hat{\varepsilon}_k^a = 2sJ^l u^l \varepsilon_k + mJu\mu^l$$
$$\hat{\varepsilon}_k^b = 2mJ^{it} u^{it} \varepsilon_k + sJu\mu^{it} \qquad (38)$$

The renormalized spin-wave theory is reproduced when $\mu^l = \mu^{it} = 1(\lambda^l = \lambda^{it} = 0)$. We assume μ^l and μ^{it} to be positive ($\mu^l > 0$, $\mu^{it} > 0$). Then, $\hat{\varepsilon}_k^a > 0$, $\hat{\varepsilon}_k^b > 0$, and $\hat{E}_k^\alpha > 0$ for all values of the wave-vector k. The β_k dispersion is non-negative, $\hat{E}_k^\beta \geq 0$ if $\mu^l \mu^{it} \geq 1$. In the particular case $\mu^l \mu^{it} = 1$ $\hat{E}_0^\beta = 0$, and, near the zero wave vector, $\hat{E}_k^\beta \approx \hat{\rho}k^2$ with spin-stiffness constant equals

$$\hat{\rho} = \frac{s^2 J^l u^l \mu^{it} + m^2 J^{it} u^{it} \mu^l}{s\mu^{it} + m\mu^l}. \qquad (39)$$

Hence, in this case, β_k boson is the long-range excitation (magnon) in the system. In the case $\mu^l \mu^{it} > 1$, both α_k boson and β_k boson are gapped excitations.

The parameters λ^l and λ^{it} (μ^l, μ^{it}) are introduced to enforce the spontaneous magnetizations of the localized and itinerant electrons to be equal to zero in the paramagnetic phase. One finds out the parameters μ^l and μ^{it},

as well as the Hartree-Fock parameters, as functions of temperature, solving the system of five equations, equations (29) and the equations $M^l = M^{it} = 0$, where the spontaneous magnetizations have the same representation as equations (30) but with coefficients $\cos\hat{\theta}_k$, $\sin\hat{\theta}_k$, and dispersions $\hat{E}_k^\alpha$, $\hat{E}_k^\beta$ in the expressions for the Bose functions. The numerical calculations show that for high enough temperature $\mu^l \mu^{it} > 1$. When the temperature decreases the product $\mu^l \mu^{it}$ decreases, remaining larger than one. The temperature at which the product becomes equal to one ($\mu^l \mu^{it} = 1$) is the Curie temperature.

Below T_C, the spectrum contains magnon excitations, thereupon $\mu^l \mu^{it} = 1$. It is convenient to represent the parameters in the following way:

$$\mu^{it} = \mu, \qquad \mu^l = 1/\mu. \qquad (40)$$

In the ordered phase magnon excitations are the origin of the suppression of the magnetization. Near the zero temperature their contribution is small and at zero temperature spontaneous magnetizations M^l and M^{it} reach their saturations ($M^l = s$, $M^{it} = m$). On increasing the temperature magnon fluctuations suppress the magnetization of localized and itinerant electrons in different ways. At T^* the magnetization of the itinerant electrons M^{it} becomes equal to zero. Increasing the temperature above T^*, M^{it} should be zero. This is why we impose the condition $M^{it}(T) = 0$ if $T > T^*$. For temperatures above T^*, the parameter μ and the Hartree-Fock parameters are solution of a system of four equations, equations (29) with $\cos\hat{\theta}_k$, $\sin\hat{\theta}_k$, $\hat{\varepsilon}_k^a$, $\hat{\varepsilon}_k^b$, $\hat{E}_k^\alpha$, $\hat{E}_k^\beta$ instead of $\cos\theta_k$, $\sin\theta_k$, ε_k^a, ε_k^b, E_k^α, E_k^β, and the equation $M^{it} = 0$. The Hartree-Fock parameters, as a functions of temperature T/J, are depicted in figure 2 for parameters $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$. The vertical dotted (green) line corresponds to T^*/J. The function $\mu(T/J)$ is depicted in figure 3 for the same parameters.

One utilizes the obtained functions $\mu(T)$, $u^l(T)$, $u^{it}(T)$, $u(T)$ to calculate the spontaneous magnetization as a function of the temperature. Above T^*, the magnetization of the system is equal to the magnetization of the localized electrons. For the same parameters as above the functions $M^l(T/J)$ and $M^{it}(T/J)$ and $M(T/J) = M^l(T/J) + M^{it}(T/J)$ are depicted in figure 4. The upper (black) line is the magnetization of localized electrons $M^l(T/J)$, the middle (red) line is the magnetization of the itinerant electrons $M^{it}(T/J)$ and the bottom (blue) line is the total magnetization $M(T/J)$. Comparing figure 4, in the present paper, and figure 2 in [1] one becomes aware of the relevance of the present calculations for the accurate reproduction of the basic features of the system near the characteristic temperatures T_C and T^*.
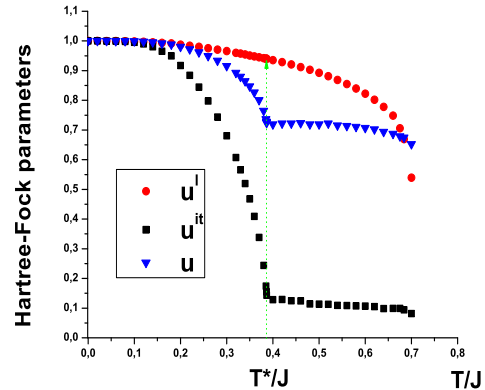

FIG. 2: (color online) Hartree-Fock parameters u^l, u^{it} and u as a function of T/J for $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$. The vertical dotted (green) line corresponds to T^*/J
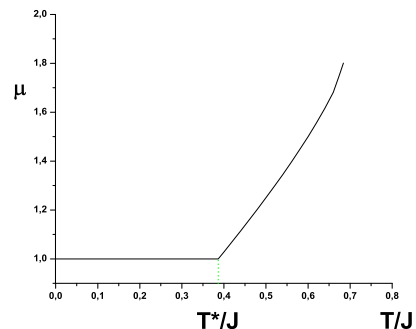

FIG. 3: (color online) $\mu(T/J)$ for parameters $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$. The vertical dotted (green) line corresponds to T^*/J

IV. THEORY AND EXPERIMENT

The present paper is inspired from the experimental measurements of the magnetization-temperature curves of UGe_2 [13, 14]. The existence of the characteristic temperature T_x in the experimental measurements and the present results (figure 4) refer us for assumption that the magnetic properties of UGe_2 are result of two magnetic moments. One can write an effective Hamiltonian in terms of two vector fields $\mathbf{M}_{1i}$ and $\mathbf{M}_{2i}$ which identify the local orientation of the magnetizations (see Eq.9)

$$h = -J_1 \sum_{\langle ij \rangle} \mathbf{M}_{1i} \cdot \mathbf{M}_{1j} - J_2 \sum_{\langle ij \rangle} \mathbf{M}_{2i} \cdot \mathbf{M}_{2j} - J \sum_i \mathbf{M}_{1i} \cdot \mathbf{M}_{2i}. \qquad (41)$$

The exchange constants J_1, J_2 and J are positive (ferromagnetic).

Magnetism of UGe_2 is due to magnetic ordered moments of $5f$ uranium electrons. They have dual char-

This fixes the exchange constant J. The constants J_1/J and J_2/J are chosen so that the ratio T_C/T^* to be close to the experimental value.
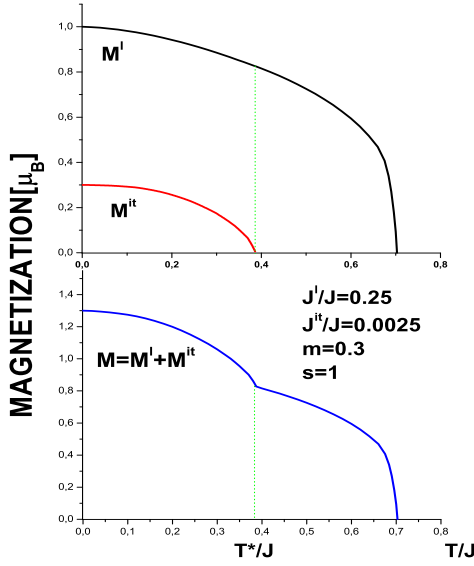

FIG. 4: (color online) The magnetization of localized electrons $M^l(T/J)$-upper (black)line, the magnetization of the itinerant electrons $M^{it}(T/J)$-middle (red) line and the total magnetization $M(T/J)$-bottom (blue) line as a function of T/J for parameters $s = 1$, $m = 0.3$, $J^l/J = 0.25$ and $J^{it}/J = 0.0025$. T^*/J- vertical dotted (green) line
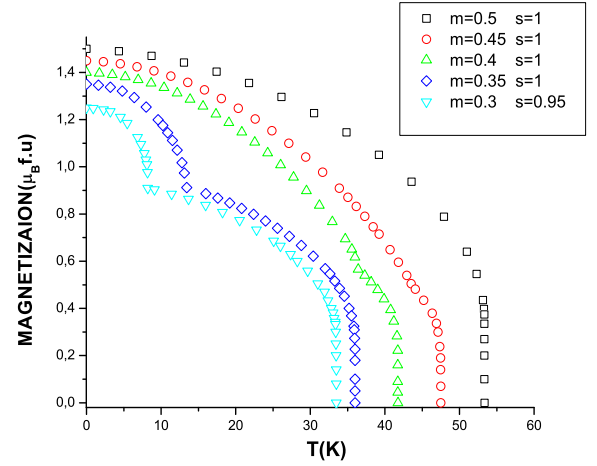

FIG. 5: (color online) Magnetization-temperature curve obtained within an effective two magnetic ordered moments model of UGe_2 magnetism

acter and in UGe_2 are more itinerant than in many uranium compounds known as "heavy-fermion systems". The $LDA+U$ calculations show the existence of well separated majority spin state with orbital projection $m_l = 0$ [17]. This can be modeled with spin 1/2 fermion. Then the local magnetization of the fermion $\mathbf{M}_{1i}$ is identical to $\mathbf{M}_i^{it}$ in the Hamiltonian Eq.9. The saturation magnetization m is close to $1/2$ at ambient pressure and decreases with increasing the pressure. The collective contribution of the others uranium $5f$ electrons to the magnetization is described by $\mathbf{M}_{2i}$ vector with saturation magnetization $s = 1$. One thinks of these electrons as localized, but they are not perfectly localized in UGe_2. This means that saturation magnetization s could be smaller then one.

The UGe_2 compounds have strong magnetic anisotropy. It can be effectively accounted for introducing a gap in the expressions for the dispersions Eq.(21) . As a result the magnon of the system has a gap. This is not important for the anomaly because it is a consequence of a different interactions of the magnon with the transversal fluctuations of the magnetization vectors $\mathbf{M}_{1i}$ and $\mathbf{M}_{2i}$. This is why the magnetic anisotropy is not accounted for. In this way I focus on the essential ingredients which lead to the anomaly.

To proceed one uses the Holstein-Primakoff representation Eqs (12) for the vectors $\mathbf{M}_{1i}$, $\mathbf{M}_{2i}$ and accomplishes the same calculations as in Section III. The obtained magnetization-temperature curves, for different choices of model parameters, are depicted in figure 5. I set the Curie temperature to be equal to the experimental one.

The first curve from above (black squares) is calculated for parameters $m = 0.5$, $s = 1$, $J_1/J = 0.0005$ and $J_2/J = 0.05$. The strong interaction between itinerant and "localized" electrons aligns their magnetic orders so strong that they become zero at one and just the same temperature T_C. The magnetization-temperature curve is typical Curie-Weiss curve. The result is different if the exchange constant J is relatively smaller. The ferromagnetic phase is divided into two phases: low temperature phase $0 < T < T^*$ where all $5f$ uranium electrons give contribution to the magnetization, and high temperature ferromagnetic phase $T^* < T < T_C$ where the contribution to the magnetization of itinerant electrons is zero. The next curve (red circles) is obtained for parameters $m = 0.45$, $s = 1$, $J_1/J = 0.0016$, $J_2/J = 0.16$, the third one (green triangles) for parameters $m = 0.4$, $s = 1$, $J_1/J = 0.0018$ and $J_2/J = 0.18$, the fourth curve (blue rhombs) corresponds to parameters $m = 0.35$, $s = 1$, $J_1/J = 0.004$ and $J_2/J = 0.4$, and for the last one $m = 0.3$, $s = 0.95$, $J_1/J = 0.0057$ and $J_2/J = 0.57$. The curves show that increasing the constants J_1/J and J_2/J the ration T_C/T^* increases ($T_C/T^* = 1, 1.092, 1.46, 2.68, 4.08$), and T^* approaches to zero ($T^* = 53.35K, 43.511K, 36.433K, 13.44K, 8.21K$). Comparing with experiments [12, 14] one concludes that increasing the pressure the exchange constant between itinerant and "localized" electrons J increases, but exchange constants between itinerant electrons J_1 and between localized electrons J_2 increase faster, so that the ratios J_1/J and J_2/J increase.

The anomalous temperature dependence of the ordered moment, known from the experiments with UGe_2 [11, 13–15], is very well reproduced theoretically in the present paper (figure 5). Below T_x (T^* in the present paper) the ferromagnetic moment increases in an anomalous way. The low temperature, large moment phase is referred to as $FM2$, while the high temperature low-momenta phase is referred to as $FM1$ [15, 18]. The present theoretical result gives new insight into $FM1 \rightarrow FM2$ transition. It is shown that between Curie temperature and $T^* < T_C$ the contribution of the itinerant UGe_2 electrons to the magnetization is zero. They start to form magnetic moment at T^*.

There are experiments which support the present theoretical result. The measurements [13] show that the resistivity display a down-turn around $T^*(= T_x)$, that is best seen in terms of a broad maximum in the derivative $d\rho/dT$ [19]. It is well known that the onset of magnetism in the itinerant systems is accompanied with strong anomaly in resistivity [20]. The experiments [13, 19] prove that only part of $5f$ uranium electrons start to form magnetic order at Curie temperature. The other ones do this at temperature $T_x(= T^*)$ well below T_C, in agreement with the theoretical result. Further evidence for the nature of the $FM1 \rightarrow FM2$ transition has been observed in the high resolution photoemission, which show the presence of a narrow peak in the density of states below E_F that suggests itinerant ferromagnetism [21].

V. SUMMARY

In summary, it is obtained an effective theory of two magnetic ordered vectors from spin-Fermion model. I have worked out a renormalized spin-wave theory and its extension to describe the two ferromagnetic phases of a spin-Fermion system: high temperature phase $T^* < T < T_C$, where only localized spins form magnetic moment, and low temperature phase $0 < T < T^*$, where localized spins and itinerant electrons contribute the ordered ferromagnetic moment.

It is important to stress that the two ferromagnetic phases can not be obtained within RKKY theory because it utilizes only the transversal fluctuations of the localized spins. Integrated over the spinless Fermions we obtain the exchange interaction between transversal fluctuations of the localized and itinerant spins instead of RKKY exchange. This point is basic for the understanding of the two ferromagnetic phases in the spin-Fermion systems.

The present theory of magnetism permits to consider more complicated systems such as the UGe_2 compound. The effective model, in terms of two magnetic ordered moments, reproduces very well the experimental magnetization-temperature curves. The results give new understanding of the two ferromagnetic phases. The large moment phase ($FM2$) is a phase where all $5f$ uranium electrons contribute the magnetization, while the electrons are partially ordered in the low-momenta phase ($FM1$). The result differs from scenarios studied in the literature [22–24], and is important for the study of the coexistence of ferromagnetism and superconductivity in these compounds.

VI. ACKNOWLEDGMENTS

Appendix A

To make more transparent the derivation of the Hamiltonian in the Hartree-Fock approximation Eq.(16) I consider the first term in the Hamiltonian of the magnon-magnon interaction Eq.(15). To write this term in the Hartree-Fock approximation one represents the product of two Bose operators in the form

$$a_i^+ a_j = a_i^+ a_j - <a_i^+ a_j> + <a_i^+ a_j> \qquad (A1)$$

and neglects all terms $(a_i^+ a_j - <a_i^+ a_j>)^2$ in the four magnon interaction Hamiltonian. The result is

$$\frac{1}{2}a_i^+ a_j a_i^+ a_i \approx -<a_i^+ a_j><a_i^+ a_i>$$
$$+ <a_i^+ a_j> a_i^+ a_i + a_i^+ a_j <a_i^+ a_i>$$

$$\frac{1}{2}a_j^+ a_i a_j^+ a_j \approx -<a_j^+ a_i><a_j^+ a_j>$$
$$+ <a_j^+ a_i> a_j^+ a_j + a_j^+ a_i <a_j^+ a_j>$$

$$\frac{1}{2}a_j^+ a_j a_i^+ a_j \approx -<a_j^+ a_j><a_i^+ a_j> \qquad (A2)$$
$$+ <a_j^+ a_j> a_i^+ a_j + a_j^+ a_j <a_r^+ a_j>$$

$$a_i^+ a_i a_j^+ a_j \approx -<a_i^+ a_i><a_j^+ a_j>$$
$$+ <a_i^+ a_i> a_j^+ a_j + a_i^+ a_i <a_j^+ a_j>$$
$$- <a_i^+ a_j><a_j^+ a_i>$$
$$+ <a_i^+ a_j> a_j^+ a_i + a_j^+ a_i <a_i^+ a_j>$$

The Hartree-Fock approximation of this part of the Hamiltonian of magnon-magnon interaction reads

$$\frac{1}{4}J^l \sum_{<ij>} \left[a_i^+ a_j^+ (a_i - a_j)^2 + (a_i^+ - a_j^+)^2 a_i a_j \right]$$

$$\approx 3NJ^l s^2 \left(u^l - 1 \right)^2 \qquad (A3)$$

$$+ sJ^l \left(u^l - 1 \right) \sum_{<ij>} \left(a_i^+ a_i + a_j^+ a_j - a_j^+ a_i - a_i^+ a_j \right)$$

where the Hartree-Fock parameter u^l is defined by the equation

$$u^l = 1 - \frac{1}{3s}\frac{1}{N} \sum_k \varepsilon_k <a_k^+ a_k> \qquad (A4)$$

Combining the a-bosons' part of the Hamiltonian Eq.(14) (the first term) and Eq.(A3) one obtaines the Hartree-Fock approximation for the a-bosons' part of the Hamiltonian Eqs.(17,18).

$$H^a \approx 3NJ^l s^2 \left(u^l - 1\right)^2 \tag{A5}$$
$$+ \; sJ^l u^l \sum_{<ij>} \left(a_i^+ a_i + a_j^+ a_j - a_j^+ a_i - a_i^+ a_j\right)$$

In the same way one obtains the Hartree-Fock approximation of the b-bosons' and inter bosons' parts of the Hamiltonian. The result is the h_{HF} Hamiltonian Eqs.(17,18).

To calculate the thermal average $< a_k^+ a_k >$, in the Eq.(A4), one utilizes the Hamiltonian h_{HF}. Therefor, the matrix element depends on the Hartree-Fock parameters, and equation (A4) is one of the self consistent equations for these parameters.

The matrix element can be represented in terms of $\alpha_k(\alpha_k^+)$ and $\beta_k(\beta_k^+)$ by means of equations(22)

$$< a_k^+ a_k > = \cos^2 \theta_k \, n_k^\alpha + \sin^2 \theta_k \, n_k^\beta \tag{A6}$$

where $n_k^\alpha = < \alpha_k^+ \alpha_k >$, $n_k^\beta = < \beta_k^+ \beta_k >$ are the Bose functions of α and β excitations. Substituting the thermal average in Eq.(A4) with Eq.(A6), one obtains that equation (A4) is exactly the first equation of the system Eq.(29) which in turn is obtained from the first of the equations (28).

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